More Accurate Finite Differences

Previously we considered the simplest finite difference approximation to *df/dx*, formulated via a Taylor Series expansion about *x*:

$$\frac{df}{dx} \equiv \frac{f(x+\Delta x) - f(x)}{\Delta x} + E \tag{1}$$

Where:

$$E \equiv True\ Error \equiv -\tfrac{1}{2}\Delta x \cdot \frac{d^2 f}{dx^2} - \tfrac{1}{3!}\Delta x^2 \cdot \frac{d^3 f}{dx^3} - \tfrac{1}{4!}\Delta x^3 \cdot \frac{d^4 f}{dx^4} - \cdots \tag{2}$$

Recall that this approximation is $O(\Delta x)$, because of the first term in the error formula involving the second derivative of $f(x)$. If we could somehow remove this term, then we can achieve a faster convergence **and** higher accuracy. The only way to do this is to consider a second expansion to a second point. Consider the Taylor Series expansion "backwards" to x-Δx instead:

$$f(x-\Delta x) \equiv f(x) - \Delta x \cdot \frac{df}{dx} + \tfrac{1}{2}\Delta x^2 \cdot \frac{d^2 f}{dx^2} - \tfrac{1}{3!}\Delta x^3 \cdot \frac{d^3 f}{dx^3} + \tfrac{1}{4!}\Delta x^4 \cdot \frac{d^4 f}{dx^4} - \cdots \tag{3}$$

Note that Δx is always taken as a positive number (it is a "step size"), and so the expansion (3) looks just like the case for x+Δx, except that the odd-power terms are subtracted rather than added. For the "forward" expansion we had:

$$f(x+\Delta x) \equiv f(x) + \Delta x \cdot \frac{df}{dx} + \tfrac{1}{2}\Delta x^2 \cdot \frac{d^2 f}{dx^2} + \tfrac{1}{3!}\Delta x^3 \cdot \frac{d^3 f}{dx^3} + \tfrac{1}{4!}\Delta x^4 \cdot \frac{d^4 f}{dx^4} + \cdots \tag{4}$$

If we subtract (3) from (4) we get:

$$f(x+\Delta x) - f(x-\Delta x) \equiv 2\Delta x \cdot \frac{df}{dx} + \tfrac{2}{3!}\Delta x^3 \cdot \frac{d^3 f}{dx^3} + \tfrac{2}{5!}\Delta x^5 \cdot \frac{d^5 f}{dx^5} + \cdots \tag{5}$$

So all odd-power terms double, while all even-power terms cancel. Re-arranging (5):

$$\frac{df}{dx} \equiv \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + E \tag{6}$$

Where:

$$E \equiv True\ Error \equiv -\tfrac{1}{3!}\Delta x^2 \cdot \frac{d^3 f}{dx^3} - \tfrac{1}{5!}\Delta x^4 \cdot \frac{d^5 f}{dx^5} - \cdots \tag{7}$$

Thus, the ***3-point central difference approximation*** (6) is $O(\Delta x^2)$, an improvement over the simpler ***2-point forward approximation*** in (1). The approximation is referred to as *3-point* because it involves the three values x-Δx, x, and x+Δx; and *central* because the expansion points are on both sides of *x*. We could also combine the following forward expansion with (4) instead:

$$f(x+2\Delta x) \equiv f(x) + 2\Delta x \cdot \frac{df}{dx} + \tfrac{1}{2}(2\Delta x)^2 \cdot \frac{d^2 f}{dx^2} + \tfrac{1}{3!}(2\Delta x)^3 \cdot \frac{d^3 f}{dx^3} + \cdots \qquad (8)$$

Now to remove the term with the second derivative we must combine $4 \cdot$ eqn(4) - eqn(8):

$$4f(x+\Delta x) - f(x+2\Delta x) \equiv 3f(x) + 2\Delta x \cdot \frac{df}{dx} - \tfrac{4}{3!}\Delta x^3 \cdot \frac{d^3 f}{dx^3} + \cdots \qquad (9)$$

Re-arranging, we get a ***3-point forward difference approximation*** to *df/dx*, also $O(\Delta x^2)$:

$$\frac{df}{dx} \equiv \frac{-3f(x) + 4f(x+\Delta x) - f(x+2\Delta x)}{2\Delta x} + \tfrac{2}{3!}\Delta x^2 \cdot \frac{d^3 f}{dx^3} - \cdots \qquad (10)$$

In summary, more accurate finite difference approximations can be formulated by taking more points for Taylor Series expansion, and combining as needed. Furthermore, the same process can be used to approximate higher-order derivatives as well. As a general rule, if you want to approximate an N^{th}–order derivative, you must use at least an (N+1)-point approximation in order to cancel the lower-order terms; but you may choose to use more points for better accuracy and convergence.

Refer to the handout *Survey of Difference Approximations* for these and other results…

Refer to Example #4 for a comparison of multi-point approximations…